Idoxuridine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.89e-10 mmHg

Global applicability domain: Outside

Local applicability domain index: 2.61e-01

Confidence level: 2.42e-01

Nearest Neighbors from the Training Set

Image not found
MCPB ethyl
Measured: 7.50e-10
Predicted: 1.69e-05

Image not found
2-Pentene, 2,3-dimethyl-
Measured: 3.00e-09
Predicted: 59.3

Image not found
Buminafos [ISO]
Measured: 2.30e-11
Predicted: 3.69e-04

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Quinalphos
Measured: 1.00e-11
Predicted: 3.29e-06

Image not found
Butanedinitrile, ethyl-
Measured: 3.70e-09
Predicted: 1.62e-02